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Crystal field theory and electric field gradients at 49Ti nuclei sites in LaTiO3

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Abstract

The energy level diagram and the wave functions for the Ti3+ ions (3d1) in LaTiO3 are calculated using modern crystal-field theory. The relative orbital ordering of these ions in the ground state is obtained. It turns out that the states of the ground triplet are considerably split and therefore the effect of the electronic-vibrational interaction is suppressed despite the fact that the distortions of the TiO 6 building block seem to be small. The components of the electric field gradient tensor at the Ti3+ nuclei sites are calculated using the wave functions of the ground states obtained. The calculated asymmetry parameter agrees well with the experimental values, which demonstrates the adequacy of the proposed orbital-ordering pattern of the Ti3+ ions in the ground state. © 2007 Pleiades Publishing, Ltd.

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